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Effect of lateral boundary conditions on electron states in tunnel-coupled quantum wells

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Abstract. The electron transport in tunnel-coupled, double-layer nanostructures of a finite size is studied theoretically. The boundary conditions for matrix distribution function of the electrons near edges and contacts are derived. The quantum size effects, associated with the tunnel coherence length, are demonstrated for several kinds of planar, laterally-restricted double-layer systems.

Introduction

The fabrication of nanostructures based upon two-dimensional (2D) electron layers assumes lateral restriction of 2D electron gas as well as creation of contacts to it. Thus, two types of boundaries, the edges and the contacts, are present in a finite-size 2D system. An investigation of electrical properties of such a system requires a knowledge of boundary conditions for both kinds of boundaries and applications of the boundary conditions to description of the distribution function of the electrons.

In this paper we derive the boundary conditions for double-layer 2D electron systems [1]. A considerable experimental and theoretical interest to these systems is concerned with manifestations of an extra degree of freedom due to the tunnel coupling of electron states. Mathematically, it means that the Hamiltonian of the system is represented by 2×2 matrix in the left (l) and right (r) layer basis. As a consequence, the distribution function of the electrons is also a 2×2 matrix, and the boundary conditions for this function should be of a matrix form. Below we obtain the boundary conditions for columnar wave functions at contacts and edges. Then, we derive the boundary conditions for the matrix Wigner distribution function. Finally, we apply these boundary conditions to calculations of the electric current along a narrow strip [2] formed from a double-layer 2D system and across narrow double-layer regions formed by independently contacted 2D layers [3].

1 Wave functions of finite-size double-layer systems

Consider a double-layer system confined in y direction. The free-particle Hamiltonian of the system is written as

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{p_x^2}{2m} + \hat{h}. \qquad (1)$$

Here p_x is the electron momentum along $0X$, and $\hat{h} = (\Delta/2)\hat{\sigma}_z + T\hat{\sigma}_x$ is the potential energy matrix expressed through the Pauli matrices $\hat{\sigma}_i$, Δ is the splitting energy in the absence of tunnel coupling, and T is the tunneling matrix element. The two-component wave function of the Hamiltonian (1) is given by

$$\Psi(y) = \mathcal{G}_+[A_1 e^{ik_+y} + A_2 e^{-ik_+y}] + \mathcal{G}_-[B_1 e^{ik_-y} + B_2 e^{-ik_-y}]. \qquad (2)$$

Here $\mathcal{G}_{\pm}$ are the columns determined by parameters Δ and T, and $k_{\pm}^2 = [2m(\varepsilon \mp \Delta_T/2) - p_x^2]/\hbar^2$ ($\Delta_T = \sqrt{\Delta^2 + (2T)^2}$ is the splitting energy of the tunnel-coupled states). The columns $\mathcal{G}_{\pm}$ describe symmetrized $\mathcal{G}_+$ and antisymmetrized $\mathcal{G}_-$ electronic states, and $\Psi(y)$ contains a linear combination of these two states.

The coefficients A_1, A_2, B_1, and B_2 are to be found from boundary conditions. For a boundary at $y = y_0$ they are given by the matrix boundary condition of third kind:

$$\left[\frac{\partial}{\partial y} + \hat{\mathcal{P}}\right] \Psi(y)\bigg|_{y=y_0} = 0. \tag{3}$$

Here $\hat{\mathcal{P}}$ is a diagonal matrix: $\hat{\mathcal{P}} = q_l\hat{P}_l + q_r\hat{P}_r$, where $\hat{P}_l = (1 + \hat{\sigma}_z)/2$ and $\hat{P}_r = (1 - \hat{\sigma}_z)/2$ are the projection matrices. The complex constants q_l and q_r, characterizing the boundary, depend on the electron momentum. They are different from each other, because the boundary potentials for different layers are different. An explicit expression of $q_{l,r}$ for a model of hard-wall edge potentials is presented in [2]. According to Eq.(3), the total microscopic current through the boundary is equal to $(i\hbar/2m)\Psi^+(y_0)(\hat{\mathcal{P}} - \hat{\mathcal{P}}^+)\Psi(y_0)$. Therefore, if the boundary is an edge (no current through it), both q_l and q_r are real. If the boundary is a contact, q_l and/or q_r contain imaginary parts proportional to the microscopic currents injected in proper layer. In practice, the contact can be made independently to l or r layer. If only l (or r) layer is contacted, we have $Im\ q_r = 0$ (or $Im\ q_l = 0$). Different kinds of structures can be realized experimentally by means of independent contacting [1,4]; two of them are shown in Fig. 1 (see also [3]).

2 Boundary conditions for Wigner distribution function

The density matrix of electrons obeys the quantum kinetic equation $\partial\hat{\rho}/\partial t + (i/\hbar)[\hat{H}, \hat{\rho}] = 0$, where $\hat{H}$ is the Hamiltonian of the system. If one uses the two-coordinate representation of the density matrix, $\hat{\rho} = \hat{\rho}_{p_x}(y_1, y_2)$, the boundary conditions for it directly follow from Eq.(3), provided that the motion of electrons across the edge or contact area is nearly ballistic:

$$\left[\frac{\partial}{\partial y_1}\hat{\rho}_{p_x}(y_1, y_2) + \hat{\mathcal{P}}\hat{\rho}_{p_x}(y_1, y_2)\right]_{y_1=y_0} = 0,$$
$$\left[\frac{\partial}{\partial y_2}\hat{\rho}_{p_x}(y_1, y_2) + \hat{\rho}_{p_x}(y_1, y_2)\hat{\mathcal{P}}^+\right]_{y_2=y_0} = 0. \tag{4}$$

For a finite-size system whose width is large in comparison with the quantum length (i.e. with the wavelength of an electron at the Fermi level), it is more convenient to introduce Wigner representation of the density matrix. Then, the quantum kinetic equation reduces to a quasi-classical kinetic equation for Wigner distribution function $\hat{f}_{p_xp_y}(y)$, provided that this function changes on the lengths larger then the quantum length. Such conditions are realized in a double-layer system when the splitting energy Δ_T is small in comparison with the Fermi energy ε_F. Assuming this, we derive the boundary condition for $\hat{f}_{p_xp_y}(y)$:

$$(ip_y + \hbar\hat{\mathcal{P}})\hat{f}_{p_xp_y}(y_0)(-ip_y + \hbar\hat{\mathcal{P}}^+) = (-ip_y + \hbar\hat{\mathcal{P}})\hat{f}_{p_x-p_y}(y_0)(ip_y + \hbar\hat{\mathcal{P}}^+), \tag{5}$$

where $p_y \simeq \hbar k_+ \simeq \hbar k_-$ is the absolute value of the electron momentum along $0Y$. For a non-contacted boundary (edge), the diagonal part $f_{p_xp_y}^l(y)\hat{P}_l + f_{p_xp_y}^r(y)\hat{P}_r$ of the distribution function obeys the boundary conditions $f^{l,r}_{p_x p_y}(y_0) = f^{l,r}_{p_x - p_y}(y_0)$, which mean that both l-layer and r-layer currents through the edge are absent.

3 Some results and discussion

The boundary condition (5) can be applied to various problems of electron transport in double-layer nanostructures. To demonstrate the effect of the edges, we consider a symmetric, finite-width $(-L/2 < y < L/2)$, infinitely long $(-\infty < x < \infty)$ double-layer strip. If a weak electric field E is directed along the strip, the linearized kinetic equation for nonequilibrium part $\delta\hat{f}_{p_x p_y}(y)$ of the distribution function is

$$\frac{p_y}{m}\frac{\partial}{\partial y}\delta\hat{f}_{p_x p_y}(y) + \frac{i}{\hbar}\left[\hat{h}, \delta\hat{f}_{p_x p_y}(y)\right]_- - eE\frac{p_x}{m}\delta\left(\varepsilon_F - (p_x^2 + p_y^2)/2m\right)$$
$$= -\left[(1 + \mu\hat{\sigma}_z), \delta\hat{f}_{p_x p_y}(y)\right]_+ /2\tau \;, \qquad (6)$$

where the collision integral is expressed through the averaged scattering time τ and scattering asymmetry parameter μ, and $[...]_\pm$ denote the commutator $(-)$ and anti-commutator $(+)$. A solution of Eq.(6) together with the boundary condition (5) allows to find the resistivity of the system. The edge effects dramatically modify the resistivity of the strip in comparison with the resistivity of a double-layer plane [5], provided that the scattering in is non-symmetric $(\mu \neq 0)$, and $q_l \neq q_r$. The most important qualitative modifications, as they seen from Fig. 2, are: the overall suppression and asymmetry of the resistance resonance peak [5], and the oscillations of the resistivity upon the background of the peak. These phenomena can be considered as manifestations of the quantum size effect, which occurs in double-layer strips at $L \sim L_T = \hbar v_F/2T$ (v_F is the Fermi velocity). The quantum size effect is suppressed when L exceeds the mean free path length $v_F\tau$, and the resistance resonance peak becomes the same as for the double-layer plane.

To demonstrate the role of contacts, we consider the independently contacted double-layer systems shown in Fig. 1 (the layers are assumed to be infinite along $0X$). A solution of the kinetic equation together with the boundary conditions (5) with complex q_l and q_r allows to find the conductance associated with the double-layer region. The conductance for both the systems has oscillations as a function of Δ, their period is determined by $\delta\Delta_T = 2\pi\hbar v_F/L$. These oscillations are of the same origin as those shown in Fig. 2, and they are suppressed at $L > v_F\tau$.

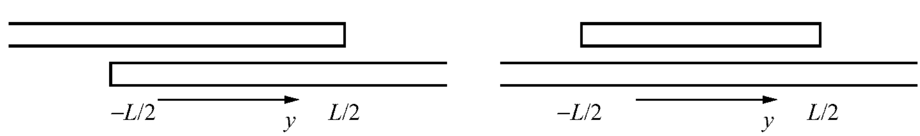

Fig 1. Two kinds of double-layer structures realized by independent contacting.

In conclusion, we have derived the matrix boundary conditions for Wigner distribution function of electrons in tunnel-coupled 2D layers, and demonstrated the quantum size effects occurring in double-layer nanostructures whose dimensions are comparable with tunnel coherence length $L_T = \hbar v_F/2T$. This length ($L_T \sim 100$ nm for typical parameters $2T \sim 1$ meV and $\varepsilon_F \sim 10$ meV) is large in comparison with the quantum

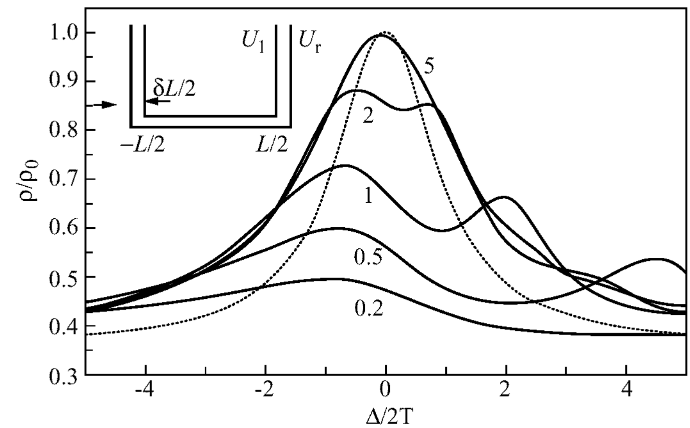

Fig 2. The shape of the resistance resonance for several values of $2TL/\hbar v_F$ (the values are shown near proper graphs) calculated in conditions $(2T\tau/\hbar)^2 \gg \mu^2$ and $v_F\tau \gg L$, at $\mu = 0.8$. The dashed line shows the same for an infinite double-layer plane. The inset shows the model of the boundaries used to estimate q_l and q_r (in the calculation we assumed that the Fermi momentum is equal to $4\hbar/\delta L$).

wavelengths of the electrons on the Fermi level. The effects could be observed experimentally in high-mobility samples at low temperatures, when the electron transport across the narrowest dimension is close to ballistic.

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